

# **Modeling Analysis of Data Captured during the CRPAQS Field Program**

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# Objective of the Project

To answer the following question: How well do air-quality models estimate measured pollutant concentrations (gaseous concentrations, total mass of  $PM_{10}$  and  $PM_{2.5}$  and mass of components of PM, etc.)?

# Proposed Modeling Tools

## CMAQ and CMAQ-MADRID

Spatial resolution: 12 km with nested 4 km grids

Vertical resolution: about 16 layers

Gas-phase chemistry: SAPRC 99

Aerosol dynamics: modal (CMAQ) and sectional  
(CMAQ-MADRID with 2, 8 and 16 sections)

Cloud and heterogeneous chemistry

Advective and diffusive transport

Dry and wet deposition



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# Model Performance Evaluation

$\text{PM}_{2.5}$  and  $\text{PM}_{10}$ , including their components  
(sulfate, nitrate, ammonium, OC, BC, etc.)

$\text{O}_3$ , NO,  $\text{NO}_2$ ,  $\text{SO}_2$  and VOC

$\text{NO}_y$ ,  $\text{NH}_3$ ,  $\text{HNO}_3$

Wet deposition fluxes



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# Model Performance Evaluation Diagnostic Analyses

Spatial and temporal scales

Effect of grid size

Vertical profiles

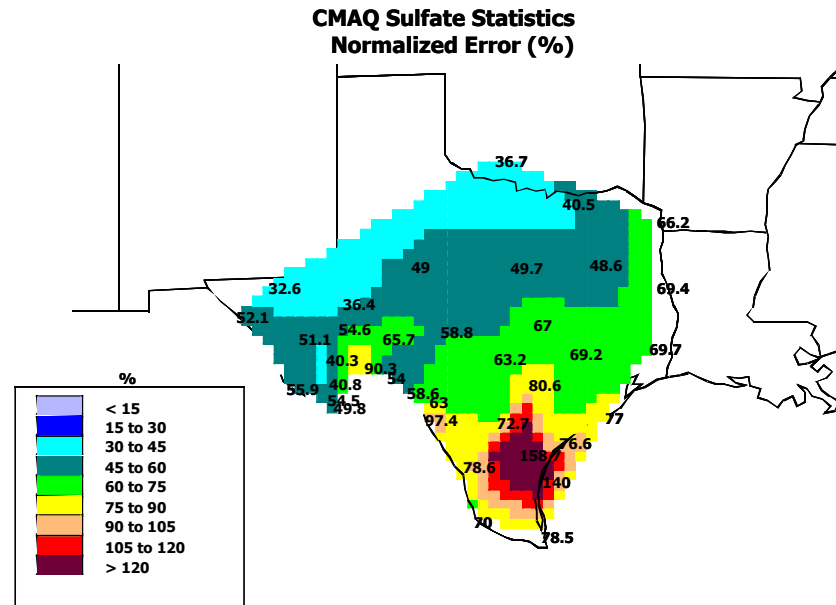
Size resolved PM

Deposition

Sensitivity analyses

# Model Performance Evaluation

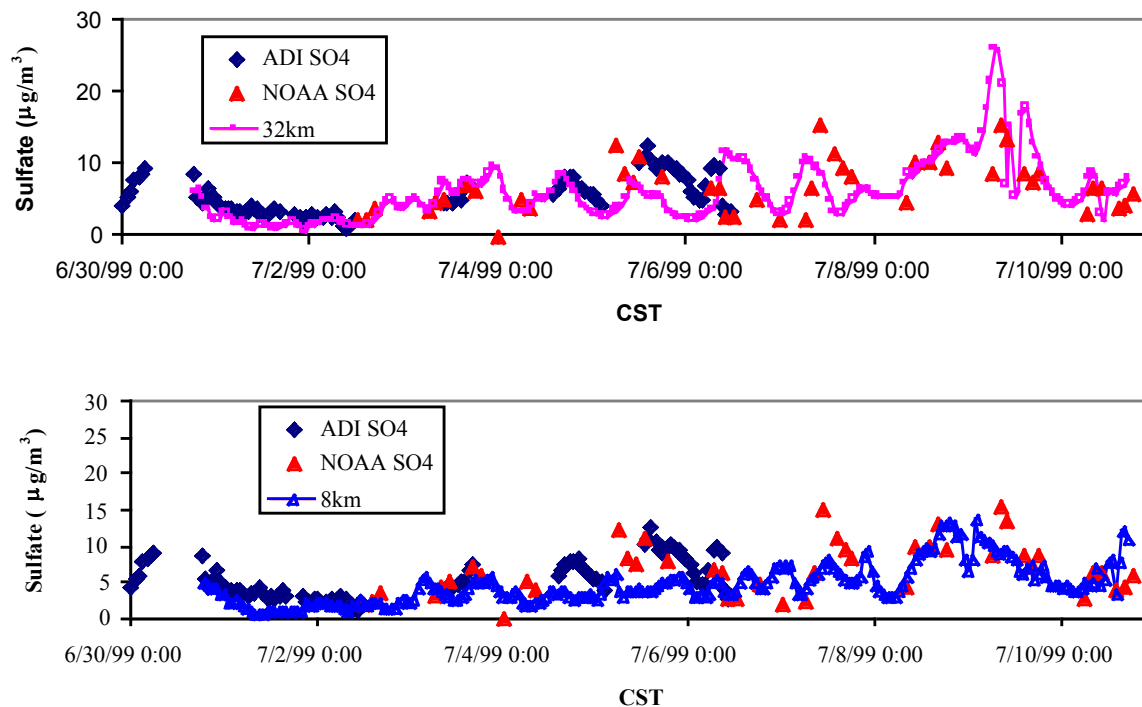
## Example of Spatial Display



Sulfate error for CMAQ-MADRID in BRAVO

# Model Performance Evaluation

## Example of Temporal Display



Observed and simulated (CMAQ-MADRID) sulfate concentrations  
in SOS99, Cornelia Fort, July 1999

# Model Simulations

Base simulation	12 km resolution
Simulation with nested grids	Two grids with 4 km resolution
PM size representations	Modal & sectional (2, 8 and 16 sizes)
Dry deposition	Algorithm of Venkatram & Pleim
Heterogeneous reactions on PM and droplets	With and without 4 heterogeneous reactions
Fog and cloud chemistry	With and without fog and cloud chemistry
Secondary organic aerosols	Different partitioning coefficients of SOA
Horizontal diffusion	Different algorithms
Vertical diffusion	Different algorithms
Photochemistry	Different photolytic rates



# Data Needs

- Inputs: Meteorology, emissions, initial and boundary concentrations and physiography
- Model performance evaluation:
  - PM (including composition) and gases
  - Fog chemistry
  - Size resolution for PM
  - Fine temporal resolution
  - Data aloft (e.g., Angiola tower)
  - Deposition fluxes